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Actinide Materials under Extreme Conditions

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During the past few years, there has been increased interest in the response of actinide-bearing materials to extreme conditions of pressure, temperature, and radiation fields. The applications span the high temperatures and pressures in the radiation fields of nuclear reactors to the formation of fission tracks in minerals deep in Earth's crust. Additionally, an understanding of the phase stability and transformation processes under these extreme conditions can be used to create a new class of materials that have novel properties or that are resistant to radiation damage.

The compressibility, phase stability, and vibrational properties of coffinite ($USiO_4$) and brannerite (UTi_2O_6) were studied by *in situ* synchrotron X-ray diffraction (XRD) and infrared (IR) measurements at high pressure up to 40 GPa. The structural behavior of brannerite is mainly characterized by a pressure-induced amorphization process, whereas in coffinite an irreversible phase transition from the zircon-type to scheelite-type structure was found to occur at 14–17 GPa [1]. However, this phase transformation in coffinite was accompanied by partial amorphization, as shown by XRD analysis. The predicted transition pressure calculated by density functional theory was in good agreement with the experimental results. The behavior of coffinite under irradiation was systematically investigated by energetic ion beam irradiation (1 MeV Kr^{2+}) and *in situ* transmission electron microscopy (TEM), which revealed a crystalline-to-amorphous transformation at a relatively low dose of ~0.27 displacements per atom (dpa) at room temperature [2].

Most recently, diamond anvil cell experiments (up to 40 GPa) have been coupled with energetic ion beams (10s of GeV) to investigate the combined effect of pressure and irradiation on $Gd_2Zr_2O_7$ pyrochlore [3]. The formation and stabilization of a new metastable high-pressure phase was observed that cannot be obtained by irradiation or pressure applied separately. TEM data and quantum-mechanical calculations suggest that these novel structural modifications are caused by the formation of nanocrystals that change the energetics of the phase transformation. This result highlights the importance of the combined use of high pressure and high-energy ion irradiation as a new means for manipulating and stabilizing novel materials to ambient conditions that otherwise could not be recovered.

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